

Quantization of non-Abelian Berry phase for time reversal invariant systems

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We present a quantized non-Abelian Berry phase for time reversal invariant systems such as quantum spin Hall effect. Ordinary Berry phase is defined by an integral of Berry's gauge potential along a loop (an integral of the Chern-Simons one-form), whereas we propose that a similar integral but over five dimensional parameter space (an integral of the Chern-Simons five-form) is suitable to define a non-Abelian Berry phase. We study its global topological aspects and show that it is indeed quantized into two values. We also discuss its close relationship with the nonperturbative anomalies.

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Quantum spin Hall (QSH) effect [1, 2, 3, 4] has attracted much renewed interest in topological order in condensed matter physics, providing us with a fundamental question about its relationship with time reversal (\mathcal{T}) symmetry. For systems with broken \mathcal{T} symmetry such as quantum Hall effect, the quantized Hall conductance is given by the TKNN integer [5], which is known to be the first Chern number [5, 6] associated with the Berry phase [7] induced in the Brillouin zone [8]. It reflects the nontriviality of the U(1) Berry phase along loops in the two dimensional Brillouin zone. Namely, it is the sum of winding numbers around vortices which are obstructions of the gauge-fixing of the wave functions.

On the other hand, for \mathcal{T} invariant systems such as QSH systems, the first Chern number is always vanishing. This does not necessarily mean that \mathcal{T} invariant insulators are topologically trivial. Recent findings are that the idea of the topological order is also crucial to the classification of \mathcal{T} invariant insulating states. The Z_2 number proposed by Kane and Mele [9, 10] for QSH effect [9, 10, 11] reveals that QSH phase is indeed a kind of topological insulator with \mathcal{T} invariance. More generically, the Z_2 number is a topological number specifying \mathcal{T} invariant systems with $\mathcal{T}^2 = -1$, where \mathcal{T} denotes the time reversal transformation as well.

Some aspects of the Z_2 number in two dimensions (2D) have become clear and its extension to 3D has been achieved [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23]. Recent success in experimental observation of evidence of the topological insulating states in HgTe [24] and in $\text{Bi}_{1-x}\text{Sb}_x$ [25, 26, 27] urges us to clarify the topological meaning of the Z_2 number. Towards this direction, it seems that topological properties in higher dimensional parameter space play a crucial role [28, 29, 30].

Another example of topological number for \mathcal{T} invariant systems is the quantized Berry phase proposed by Hatsugai [31]. While symmetry-broken phases are characterized by local order parameters, those without symmetry-breaking, which occur especially in low dimensions, can be classified by topological order parameters. The quantized Berry phase can serve as a local topological order

parameter of gapped quantum liquids. The quantized Berry phase in [7], and the use of it as a local topological order parameter [31] was proposed only for \mathcal{T} invariant systems with $\mathcal{T}^2 = 1$. Since it vanishes identically for $\mathcal{T}^2 = -1$ systems, the generalization of the idea to the latter case is an intriguing problem both in its own right and with a view to clarifying the topological meaning of the Z_2 number.

In this paper, we propose a quantized non-Abelian Berry phase for \mathcal{T} invariant systems with $\mathcal{T}^2 = -1$. This can be achieved by the use of the Chern-Simons five-form, which shares several important features with the Chern-Simons one-form for the conventional Berry phase. We show that it is indeed quantized into two values, and discuss the close relationship with the nonperturbative anomalies in field theories of Weyl fermions [32].

We first discuss a simpler case with $\mathcal{T} = \mathcal{K}$, i.e., $\mathcal{T}^2 = 1$, where \mathcal{K} denotes the operator of taking complex conjugate. Let $H(x)$ be a time reversal invariant Hamiltonian, $\mathcal{T}H(x)\mathcal{T}^{-1} = H(x)$, where x denotes a set of parameters $\{x_i\}$. In this case, Berry's gauge potential for the n multiplet $\psi(x)$ is defined as $A = \psi^\dagger d_x \psi$, where $d_x = dx_i \partial_{x_i}$ is the exterior derivative with respect to x_i . Time reversal invariance ensures that $\mathcal{T}\psi(x)$ describes the same eigenstates of $H(x)$, and hence, Berry's gauge potential for these \mathcal{T} -transformed wave functions is given by A^* . It has been shown [31] that Berry phase, which is the integral of the gauge potential over a circle S^1 in the space spanned by x ,

$$\Omega_1 \equiv \frac{i}{2\pi} \int_{S^1} \omega_1(A), \quad (1)$$

where $\omega_1(A) \equiv \text{tr } A$ is the Chern-Simons one-form, is quantized such that $\Omega_1 = 0$ or $1/2$ (in units of 2π). This can be proved by means of the following two properties: (i) ω_1 is gauge-dependent and its integral Ω_1 can be defined only mod 1. In particular, since $\mathcal{T}\psi$ and ψ denote the same eigenstates, the difference between them is just a gauge transformation, provided that ψ is normalized. (ii) ω_1 is imaginary in the following sense: $\omega_1(A^*) = -\omega_1(A)$, which can be easily seen by noting that A is

anti-Hermitian and hence, $A^* = -A^T$.

These two properties lead to the relationship $\Omega_1 = -\Omega_1 \bmod 1$, implying that Ω_1 is quantized such that $\Omega_1 = 0, 1/2 \bmod 1$ [31].

Now, we would like to show that similar techniques apply to the case $\mathcal{T}^2 = -1$, and therefore, the Z_2 invariant could be understood as a consequence of a quantized Berry phase. In this case, Berry's gauge potential is $sp(n)$ -valued, as will be discussed below, and therefore, Chern-Simons one-form is identically zero. This is true for non-Abelian gauge potential belonging to semi-simple Lie algebras. In other words, the fundamental group of a gauge group G mentioned above is trivial, $\pi_1(G)=0$. Therefore, the conventional Berry phase (1) plays no role in the case $\mathcal{T}^2 = -1$. To circumvent the difficulty, one can utilize higher forms for the present case. Here, the property of the Chern-Simons $(2n-1)$ -form ($n = 1, 2, \dots$)

$$\omega_{2n-1}(A^*) = (-)^n \omega_{2n-1}(A) \quad (2)$$

plays an important role. This tells that the Chern-Simons five-form,

$$\omega_5(A) = \text{tr} \left[A(dA)^2 + \frac{3}{2} A^3 dA + \frac{3}{5} A^5 \right],$$

is also imaginary and hence, a natural candidate giving a quantized non-Abelian Berry phase. As to the gauge dependence property (i) of the five-form, we have [33]

$$\omega_5(A_g) = \omega_5(A) + d\alpha_4(V_g, A) + \frac{1}{10} \text{tr} (g^{-1} dg)^5, \quad (3)$$

where A_g denotes the gauge transform of A , $A_g = g^{-1}Ag + g^{-1}dg$, V_g is a one-form defined by $V_g \equiv dgg^{-1}$, and α_4 is a four-form defined by

$$\begin{aligned} \alpha_4(V, A) = & -\frac{1}{2} \text{tr}[V(AF + FA)] \\ & + \frac{1}{2} \text{tr}[VA^3 + V^3 A + \frac{1}{2}(VA)^2]. \end{aligned} \quad (4)$$

Here, F is the field strength 2-form defined by $F = dA + A^2$.

These generic formulas are helpful to define a Berry phase and to show it to be quantized. Let $H(x)$ be a time reversal invariant Hamiltonian $\mathcal{T}H(x)\mathcal{T}^{-1} = H(x)$, where $\mathcal{T} = i\sigma^2\mathcal{K}$ and we assume that x stands for a set of five parameters x_i ($i = 1, \dots, 5$), since the codimension of eigenvalue degeneracies is five [28]. Let $\Psi(x)$ be a Kramers multiplet with $2n$ degenerate states

$$\Psi(x) = (\psi(x), \mathcal{T}\psi(x)).$$

Berry's gauge potential is defined by $A = \Psi^\dagger d_x \Psi$, as usual. Note that the \mathcal{T} transformation yields $\mathcal{T}\Psi(x) = \Psi(x)J$ with $J = 1_n \otimes i\tau^2$, where τ^a is the Pauli matrix operating on the space of the Kramers doublet. Then,

one finds that the gauge potential A belongs to $sp(n)$ algebra because of the relation

$$A^* = JAJ^{-1}.$$

This equation also tells that the representation of A is pseudo-real.

Since the codimension of the eigenvalue degeneracies is five, we can choose in general four dimensional sphere S^4 on which there are no such degeneracies except for the Kramers degeneracy. Inside S^4 , there could be a level-crossing of several Kramers doublets, which yield an $Sp(n)$ monopole. Consequently, the gauge potential may not be well-defined globally on S^4 ; it can only be defined on several patches: For simplicity, we assume that two hemispheres D_\pm^4 with $D_+^4 \cup D_-^4 = S^4$ are needed, and on D_\pm^4 the gauge potential is given by A_\pm , respectively. On the overlap region $D_+^4 \cap D_-^4$, they are related each other as

$$A_+ = h^{-1}A_-h + h^{-1}d_xh,$$

where $h(x)$ denotes a transition function satisfying

$$h(x) = Jh^*(x)J^{-1},$$

which, as well as the fact that h is unitary by definition, tells that h is an element of $Sp(n)$. The universality class is specified by the winding number of h over S^3 , since $\pi_3(Sp(n)) = \mathbb{Z}$. This winding number is nothing but the second Chern number discussed in [28]. Here, the difference of the Chern-Simons three-form $\omega_3(A_+) - \omega_3(A_-)$ is relevant to the integer winding number, but each three-form never gives a quantized Berry phase.

A natural integral domain for the Berry phase may be a compact manifold with dimension equal to its codimension minus one. In the previous case with $\mathcal{T}^2 = 1$, the codimension of eigenvalue degeneracies is two and the Berry phase is defined over S^1 as described in Eq. (1), whereas in the present case, the codimension is five and integral domain may be typically S^4 . Therefore, the use of the five-form for a quantized Berry phase requires another degree of freedom. This feature is analogous with the non-Abelian anomalies: These anomalies appear in four-dimensional gauge theories of Weyl fermions, but their topological meaning can be revealed in five dimensions, where one extra dimension is a parameter of the gauge transformation which defines a gauge-orbit space [34].

According to the techniques in the non-Abelian anomalies, we next introduce a one-parameter family of gauge transformations $g(x, \theta)$, where the parameter θ serves as an extra dimension. Then, provided $g(x, 2\pi) = g(x, 0)$, we can regard the gauge transformation g as being defined on a five dimensional space $S^4 \times S^1$. The gauge-transformed potential is denoted as $\mathcal{A} = g^{-1}Ag + g^{-1}dg$, where we have extended the exterior derivative d_x to

$d = d_x + d_\theta$. The transition function between \mathcal{A}_\pm , which corresponds to the gauge transform of A_\pm , respectively, is given by $\tilde{h} \equiv g^{-1}hg$. Now let us define a Berry phase which is expected to serve as a topological order for the \mathcal{T} invariant systems with $\mathcal{T}^2 = -1$;

$$\Omega_5 = \frac{i^3}{3!(2\pi)^3} \left[\int_{S^4 \times S^1} \omega_5(\mathcal{A}) - \int_{S^3 \times S^1} \alpha_4(V_{\tilde{h}}, \mathcal{A}_-) \right]. \quad (5)$$

The expression of the first term is quite formal: When one calculates this integral, one must divide S^4 into the patches D_\pm^4 and use well-defined gauge potential \mathcal{A}_\pm there, respectively. The additional second term is integrated over the boundary $\partial D_\pm^4 \times S^1 = S^3 \times S^1$. Therefore, this term may be interpreted as a boundary term which is necessary for the phase to be quantized. We will show in several steps that the phase Ω_5 is quantized for \mathcal{T} invariant systems in the similar manner as Ω_1 , and therefore, can be regarded as a non-Abelian version of Eq. (1).

Firstly, it should be noted that Ω_5 vanishes if g is kept strictly $Sp(n)$ -valued [35]. This is not surprising, because the Chern-Simons five-form has intimate relationship with the gauge anomalies, and it is well-known that the latter vanish for pseudo-real gauge potentials. However, this never means that the present gauge potential is topologically trivial: The $SU(2)$ anomaly [36, 37], or more generically, non-perturbative anomalies [38] cannot be described by local fields like Eq. (5), but by the use of the following techniques of embedding, their topologically distinct sectors can be revealed only by local gauge fields. To be concrete, the gauge transformation $g \in Sp(n)$ is embedded in $SU(2n+1)$, and the gauge potential \mathcal{A} is likewise [36, 37, 38]. Note here that the symmetry of the transition function h plays an important role in the classification of the universality class, so we impose the boundary condition that $\tilde{h} \in Sp(n)$ on $S^3 \times S^1$ when embedding g into $SU(2n+1)$. This does not necessarily mean that $g \in Sp(n)$ on the boundary: We assume that g is factorized on the boundary $S^3 \times S^1$ such that

$$g(x, \theta) = h_0(x, \theta)g_0(x, \theta), \quad (6)$$

where $h_0 \in Sp(n)$ and $g_0 \in SU(2n+1)$. Then, if g_0 is commutative with generic $Sp(n)$ elements, we have indeed $\tilde{h} \in Sp(n)$. Such g_0 is given by $g_0 = e^{i\theta\lambda/2}$ [39], where $\lambda \in su(2n+1)$ is

$$\lambda = \text{diag}(\underbrace{1, 1, \dots, 1}_{2n}, -2n).$$

The space denoted as $2n$ in the above is the space of $Sp(n)$. The normalization of λ should be chosen such that $\tilde{h}(x, 2\pi) = \tilde{h}(x, 0)$ [39]. Although the symmetry group $Sp(n)$ of the transition function is thus kept unchanged, the gauge potential itself is nontrivial even on $S^3 \times S^1$, since it has a nonzero θ component \mathcal{A}_θ through $g^{-1}d_\theta g \in su(2n+1)$.

Secondly, by making use of Eq. (3), it turns out that Eq. (5) can be written as

$$\Omega_5 = \frac{i^3}{3!(2\pi)^3} \int_{S^3 \times S^1} \tilde{\alpha}_4(h, g; A) + n_g^{(5)}, \quad (7)$$

where $n_g^{(5)}$ is a winding number of g over $S^4 \times S^1$ [40], and the four-form $\tilde{\alpha}_4$ is defined by

$$\begin{aligned} \tilde{\alpha}_4(h, g; A) &\equiv \alpha_4(V_g, A_+) - \alpha_4(V_g, A_-) - \alpha_4(V_{\tilde{h}}, A_-) \\ &= \alpha_4(V_g, v_g) - \alpha_4(V_{\tilde{h}}, v_g) - \alpha_4(V_h, A_-) + \text{t.d.} \end{aligned} \quad (8)$$

Here, the first line is the definition of $\tilde{\alpha}_4$. In the second line, $v_g \equiv g^{-1}dg$, and $\text{t.d.} \equiv d\beta_3$ with some three-form β_3 denotes the total divergence (exact form) which gives no contribution to Eq. (7). The second line can be derived from a more basic decomposition formula,

$$\alpha_4(V_{gh}, A) = \alpha_4(V_h, A_g) + \alpha_4(V_g, A) - \alpha_4(V_h, v_g) + \text{t.d.}$$

Eq. (8) tells that $\tilde{\alpha}_4$ depends on the gauge potential A only through $\alpha_4(V_h, A_-)$ as well as t.d. terms, both of which vanish by the integration in Eq. (7) [41]. Therefore, we dare to suppress the irrelevant A -dependence of $\tilde{\alpha}_4$, referring to it as $\tilde{\alpha}_4(h, g)$ for simplicity. It should be stressed that $\tilde{\alpha}_4(h, g)$ can be nonzero if and only if g depends on $\lambda \in su(2n+1)$.

The expression (7) is helpful to show that Ω_5 is indeed topological. To see this, we note that under the variation of h or g , we have

$$\delta\tilde{\alpha}_4(h, g) = \frac{1}{2}\text{tr}(\Delta_{\tilde{h}}V_{\tilde{h}}^4 - \Delta_hV_h^4) + \text{t.d.}, \quad (9)$$

where $\Delta_h \equiv \delta hh^{-1}$. It should be noted that there are no terms such as V_g ; g appears only through $\tilde{h} \in Sp(n)$. Therefore, every form V as well as the variation Δ in the above equation is strictly $sp(n)$ -valued, and hence, it vanishes identically. The other term denoted by t.d. also vanishes due to the integration, of course. We thus conclude that $\delta\Omega_5 = 0$. This implies that Ω_5 cannot change continuously. In Eq. (6), we have made a specific embedding of $Sp(n)$ into $SU(2n+1)$, but the observation here tells that as far as one imposes the boundary condition on g such that $\tilde{h} \in Sp(n)$ on $S^3 \times S^1$, one can expect that Ω_5 is quantized for any other embeddings.

Finally, we show that Ω_5 is indeed quantized under the present embedding such that $\Omega_5 = 0$ or $1/2 \bmod 1$. To this end, note the following relations

$$\begin{aligned} \tilde{\alpha}_4(h, g_1g_2) &= \tilde{\alpha}_4(h, g_1) + \tilde{\alpha}_4(g_1^{-1}hg_1, g_2) + \text{t.d.} \\ \tilde{\alpha}_4(h_1h_2, g) &= \tilde{\alpha}_4(h_1, g) + \tilde{\alpha}_4(h_2, g) + \tilde{\beta}_4(\tilde{h}_1, \tilde{h}_2), \end{aligned} \quad (10)$$

where the last term $\tilde{\beta}_4$ depends only on $\tilde{h}_j \in Sp(n)$, and therefore, it vanishes. Applying Eq. (10) to Eq. (8) with

the assumption (6), we have

$$\begin{aligned}\tilde{\alpha}_4(h, g_0 h_0) &= \tilde{\alpha}_4(h, g_0) + \tilde{\alpha}_4(g_0^{-1} h g_0, h_0) \\ &= \alpha_4(i\lambda d\theta/2, v_h) - \alpha_4(V_h, i\lambda d\theta/2) \\ &= \frac{id\theta}{2} \text{tr } v_h^3.\end{aligned}$$

Here, we have used the fact that the second term in the r.h.s. of the first line vanishes, since both h_0 and $g_0^{-1} h g_0 \in \text{Sp}(n)$. It thus turns out that Ω_5 is given by

$$\Omega_5 = \frac{1}{2} n_h^{(3)} + n_g^{(5)},$$

where $n_h^{(3)}$ is the winding number of the transition function h over S^3 . This equation tells that Ω_5 is quantized $\Omega_5 = 0, 1/2 \bmod 1$, where $\bmod 1$ comes from $n_g^{(5)}$, i.e., the winding number of g which is introduced artificially as a probe of specifying the topological sector of Berry's gauge potential defined on S^4 . It also claims the similarities between Ω_1 and Ω_5 : The former (the latter) is basically given by half the first (second) Chern number.

In summary, we have defined a quantized non-Abelian Berry phase for time reversal invariant systems with $T^2 = -1$ by the use of the Chern-Simons five-form. Although we have concentrated on global aspects of the quantized non-Abelian Berry phase, we would like to stress here that it can also serve as a local topological order parameter. Namely, for T invariant models in any dimensions, we can compute a quantized non-Abelian Berry phase as a local order parameter by adding some suitable local perturbations [31].

There still remains several important issues to be clarified. In particular, the direct relationship between Z_2 number defined in 2D Brillouin zone (T^2) [9, 15] and the quantized Berry phase defined in a five dimensional parameter space ($S^4 \times S^1$) is not yet very clear. This is mainly due to the fact that the former is inevitably calculated through the Fourier transformation which breaks time reversal symmetry in the sense that Kramers multiplet belong to opposite momentum sectors, whereas the existence of the Kramers degeneracy in the whole parameter space plays a vital role in the present formulation of the quantized Berry phase. We believe that if time reversal symmetry is broken, $\text{Sp}(n)$ monopole would split into $2n$ $U(1)$ monopoles with opposite charges, which can be detected by the Z_2 number in the Brillouin zone. However, the present formulation does not directly cover the theory of the Z_2 number.

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by the use of h_0 , $g = h_0g_0$ can recover the periodicity. However, even without this periodicity of g , we can see from Eq. (9) that the variation includes only $\tilde{h} = g^{-1}hg$, and hence the 2π -periodicity of \tilde{h} is enough to regard the space spanned by θ as S^1 .

[40] If we further impose the boundary condition $g(x, \theta =$

$0) = 1$, we can regard g as a mapping from S^5 to $SU(2n+1)$, which has a nontrivial winding number, since $\pi_5(SU(2n+1)) = \mathbb{Z}$.

[41] Note that $\alpha_4(V_h, A_-)$ does not have $d\theta$.